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Use of Artificial Neural Networks and Regression Models in Groundwater Quality Studies in the Suburbs of Aligarh City, India

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Abstract:- This study explores the application of regression models and artificial neural networks (ANNs) in predicting Total Dissolved Solids (TDS) in groundwater within two distinct regions of Aligarh city - the Northern Area Samples (NAS) and the Southern Area Samples (SAS). It aims to identify the key predictors of TDS in both areas and to compare the effectiveness of the two modelling approaches. In the NAS, sulphate, bicarbonate, sodium, and chloride were found to be the major TDS predictors, with the strongest being sulphate. In contrast, the SAS showed sodium, magnesium, potassium, and chloride as the main predictors, with sodium as the most influential. The ANN models displayed strong validity with high R square values between observed and predicted neurons. The study concluded that the ANN predictive models for TDS produced more accurate results than multilayer regression models, thereby demonstrating their broader applicability in groundwater quality characterisation and predictive modelling. The findings of this study can contribute to more effective water resource management strategies, especially in areas heavily reliant on groundwater.

Keywords:- *Predictive Modeling, Water Resource Management, Urban Sprawl,*

I. INTRODUCTION

Providing safe drinking water is a challenging task for the developing world. The task becomes more difficult in countries with a growing population, rapid urbanisation, rampant industrialisation, and extensive agricultural practices. Once groundwater quality deteriorates, its reclamation will be consequential to economic, industrial, and agricultural growth. Regular monitoring and characterisation of groundwater quality in areas with urban sprawling is necessary for sustainable development and management of shallow aquifers. Conventional graphs [1,2]), diagrams, and ratios [3,4]] are commonly used to characterise groundwater quality. The software-aided multivariate statistical tools smoothen the results of traditional graphical methods and give robust results. The advent of mathematical simulation added a predictability factor to the large set of groundwater quality data. Applicability of Artificial Neural Networks (ANN) increased significantly in all branches of sciences and engineering after the development of a mathematically rigorous theoretical framework by Rumelhart et al. [5]. The artificial neural network is gaining importance in groundwater quality studies. ANN mimics the human brain and acquires knowledge through the training process by assigning synoptic weight to the connections and values to the nodes. The ANN has applicability in hydrogeology because of its ability to solve complex problems of pattern recognition, association control, and non-linear modelling. Changes in groundwater chemistry take place from recharge to discharge zone. The local, intermediate, and regional groundwater zones bear different signatures depending on the groundwater's travel distance and depth [6]. Domestic and agricultural wastes, along with industrial effluent, impair the groundwater quality. Estimating these complex and non-linear parameters makes groundwater quality modelling problematic; thus, the application of ANN gains momentum. Kheradpisheh et al. [7] illustrated the use of back-propagation algorithms for modelling Cl, EC, SO4, and NO3 concentrations in the groundwater of the Bahabad plains of Iran. The study found it cost-effective and suitable for groundwater management practices. Khaki et al. [8] applied ANN to water quality parameters of five different locations in Langat Basin, in the southeastern part of Selangor state, Malaysia. Mean square error and sensitivity analysis showed the effectiveness of ANN in predicting TDS with low MSE values. Asadollahfardi et al. [9] showed the suitability of ANN in predicting the TDS of Talkheh Rud River water in northwest Iran. The study concluded that the Multi-layer perceptron is adequate for quick estimation of salinity. In India, the ANN model of Godavari River water quality from 2001-2012, shows that the prediction of TDS is highly accurate and valid [10]. Sinha [11] showed the efficiency of ANN in predicting the water quality index using the physicochemical parameter of groundwater quality of the Jodhpur district in the water-stressed state of Rajasthan, India. Chowdhary [12] used ANN to predict the Total dissolved Solids in the groundwater of Nadia district, West Bengal, India. The architecture of the ANN model used the three input layers (specific conductivity, chloride, and TH), twenty hidden and one output layer. The model predicted TDS with a low value of RMSE. It further elaborates on the dominance of specific conductivity and TH over chloride and potassium in predicting TDS. Urban sprawling is a global phenomenon. Migration towards urban

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centres searching for food and fibre in developing countries is unprecedented. The city sprawl is uncontrolled and unplanned. The application of ANN in predicting TDS of groundwater around the township of one million people is chosen for the present study with the following objectives. Develop the regression models and compare the models to find effective variables. Find the best topology for Artificial Neural networks. Find the suitability of the best predictive model for spatio-temporal sets of water quality data.

II. MATERIAL AND METHODS

Study Locale: The study was conducted in Aligarh city, located within the Ganga-Yamuna interfluves in the Ganga basin, India. Situated in a subtropical climatic zone, the city's geographical coordinates range from 27 28' to 28 10'N in latitude and 77 0 29’00” to 78 36’00” E longitude. The area typically receives an average rainfall of 802 mm annually and experiences temperatures ranging from 4°C in winter to 42°C in summer. With the general direction of groundwater flow from northwest to the southeast, the city relies entirely on groundwater as no surface water bodies are in the vicinity for domestic and industrial uses.

Sample Origin and Data Acquisition: The samples studied were collected from the outskirts of Aligarh city, a region anticipated to experience rapid urbanisation and densification (Fig. 1). The data used in the study were extracted from two areas, referred to as the northern area samples (NAS) and southern area samples (SAS), consisting of fifty observations. from ten distinct locations each. A total of hundred samples were collected and used in the study. Data collection took place from September 2016 to January 2017 through the use of hand pumps tapping into shallow aquifers. The IBM SPSS Statistics 20, Inc., was employed for regression analysis and for constructing Artificial Neural Network (ANN) models.

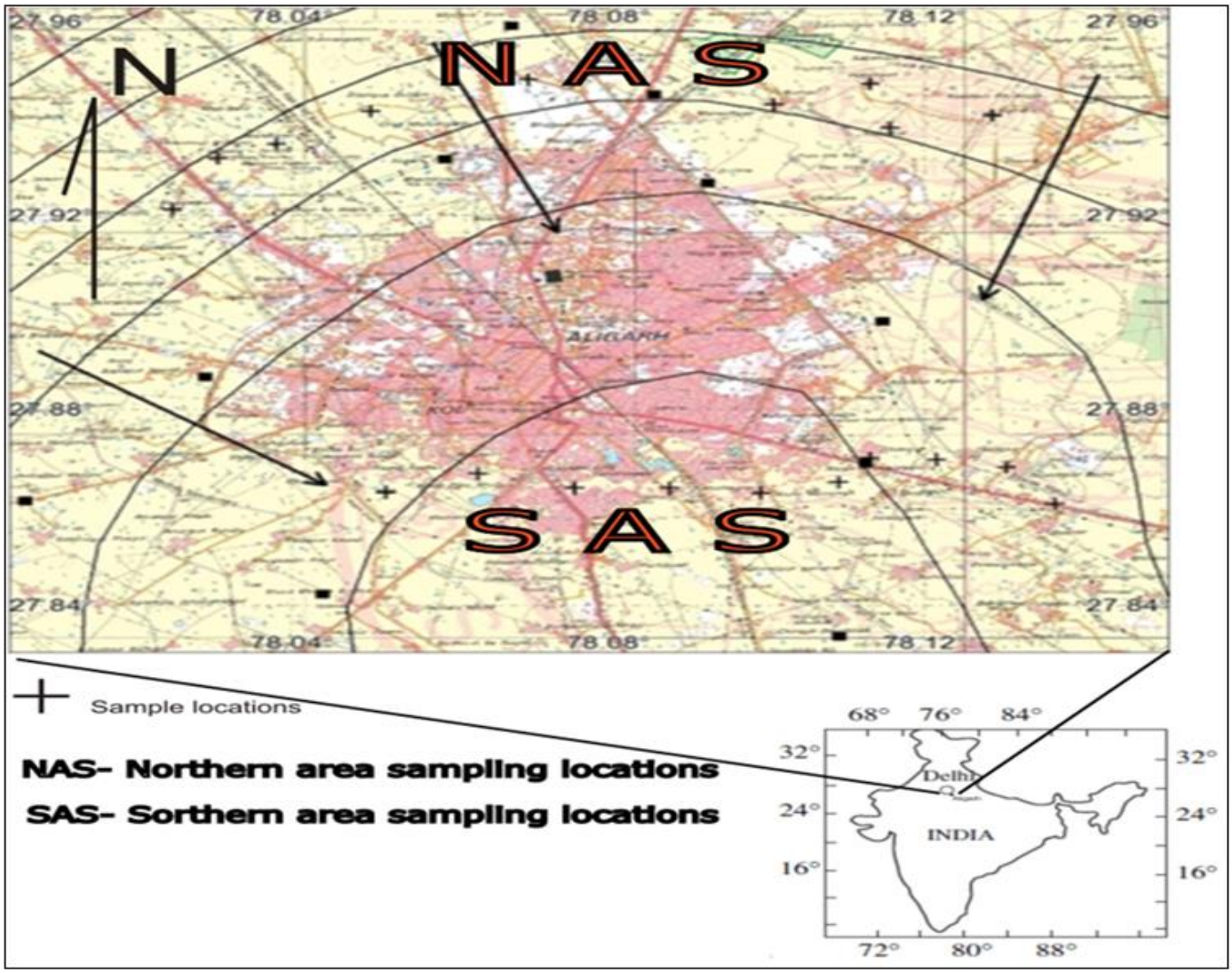

Fig 1 Location Map of the Study Area.

Aquifer Systems: The area hosts three to four interconnected aquifer tiers, leading to increased vulnerability of the underlying hydrogeologic setups. The primary aquifer, semi-confined to unconfined in nature, extends up to 120 mbgl and is comprised of thick alluvial sediments with interspersed layers of sand, clay, and silt [13] (Fig 2).

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Regression Models: Based on the least squares method, these models are effective statistical tools for identifying relationships between dependent and independent variables. Regression analysis facilitates understanding the significant variance by eliminating the less interesting variation in one variable. It also aids in predicting the value of one variable given the knowledge of others [14].

Artificial Neural Networks (ANNs): Drawing inspiration from the functioning of the human brain and nervous system, ANNs are nature-mimicking data mining techniques. Initially used for tasks like recognizing familiar faces and handwriting, the current applications extend to predicting water resources, water quality, and water levels. ANN processes information similarly to natural neural networks comprising billions of interconnected neurons. The typical ANN structure consists of input, hidden, and output layers, with weighted interconnections between the neurons. Stimulation at the input layer initiates data processing, leading to output generation [15].

The use of ANN is especially relevant for non-linear data distribution. It is advantageous because it can handle noise, outliers, small sample sizes, and accommodating non-compensatory models. The ANN algorithm initially learns through a training process using the feed-forward-backwards propagation algorithm [16].

In contrast to the pre-imposed assumptions of linear regression analysis, the neural network establishes relationships between dependent and independent variables during the learning process. If the variables are linearly related, the model adjusts accordingly. On the other hand, if the relationship is non-linear, the model assumes, corrects, and aligns appropriately. The feedforward architecture model comprises an input, hidden, and output layers.

The multilayer perceptron technique (MLP), a subset of ANN, has shown superior results compared to the Radial basis function analysis. Used primarily for classification, prediction, and recognition, MLP's architecture includes input, hidden, and output layers. Groundwater quality variables were assigned a scale measure, whereas months and locations were designated nominal or categorical. The total dissolved solids were taken as the target or dependent variables, while the rest were treated as covariates. The model allocated 70% of the samples for learning and 30% for testing. Running the MLP ten times for learning reduced errors and improved prediction accuracy [17]. This ten-fold cross-validation technique also helped prevent overfitting and obtain an average of root mean square errors (RMSE) [18].

III. RESULTS AND DISCUSSIONS

Table 1. Result summary of Regression Analysis for NAS.

Model	Unstandardized coefficientents	t	R	R- Square	Adjusted R Square	Significance
(constant	-12.058	-0.119	0.888	0.789	**0.747**	0.906
Calcium	-.362	-0.332	-	-	-	0.741
Magnesium	.587	0.510	-	-	-	0.613
Sodium	.915	**2.836**	-	-	-	**0.007**
Potassium	.535	1.557	-	-	-	.127
Carbonate	.157	.305	-	-	-	.762
Bicarbonate	.513	**2.961**	-	-	-	**.005**
Chloride	1.049	**2.826**	-	-	-	**.007**
Sulphate	.569	1.665	-	-	-	.103

In this study, the multiple regression model was employed with Total Dissolved Solids (TDS) serving as the estimator, while all the cations and anions functioned as predictors. As indicated in Table 1, which outlines the model summary, the R square value suggests that the model can account for approximately 78.9% of the variance using the major ions as response variables.

As a rule of thumb, if the t-value falls between -2 and +2, it signifies a weak relationship. However, in this analysis, a t-value greater than 2 was observed for chloride, sodium, and bicarbonate, indicating a strong relationship as corroborated by their respective p-values.

The model yields a negative intercept value (constant). However, this should not be a cause for concern, as it simply implies that the estimated value of TDS will be less than zero when the concentrations of all major ions are zero.

Taking into account 50 observations across eight variables, the multiple linear regression model for NAS can be expressed in Equation 1 as follows:

TDS = -12.058 - 0.362x (calcium) + 0.587x (magnesium) + 0.915x (sodium) + 0.535x (potassium) + 0.157 x(carbonate) + 0.513x (bicarbonate) + 1.049 x(chloride) + 0.569 x(sulphate)----------(1)

For the Southern Area Samples (SAS), the regression model yielded an R square value of 0.824 (Table 2). This implies that the predictive model accounts for a substantial proportion of the variance, with 82.4% of the variance being explained by the model itself. The coefficients of the model reveal that the variables magnesium and sodium display t values >2, with a significance level of <0.05. These two variables, therefore, make a significant contribution to explaining the results within this model.

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Table 2 Result Summary of Regression Analysis for SAS

Model	Unstandardized coefficients	t	R	R Square	Adjusted R Square	Significance
(constant	-180.373	-1.534	.908	.824	**.789**	.133
Calcium	4.894	1.989	-	-	-	.053
Magnesium	2.551	**2.638**	-	-	-	**.012**
Sodium	1.537	**4.788**	-	-	-	**.000**
Potassium	.913	1.838	-	-	-	.073
Carbonate	.440	.310	-	-	-	.758
Bicarbonate	.212	.880	-	-	-	.384
Chloride	.620	1.996	-	-	-	.053
Sulphate	.400	.834	-	-	-	.409

The multiple regression equation for the SAS, formulated from 50 samples across eight variables, is outlined in Equation 2 as follows:

TDS = -180.373 + 4.849 x (calcium) + 2.551 x (magnesium) + 1.537 x (sodium) +0.913 x (potassium) +0.440 x (carbonate) +0.212 x (bicarbonate) +0.620 x (chloride) + 0.4 x (sulphate) ----------(2)

The presence of chloride and bicarbonate in the NAS suggests that there is a recharge from a mixture of regional and local flow systems. Conversely, the SAS show no dependence on the bicarbonate variable, indicating that the groundwater quality of these samples carries signatures typical of a discharge area.

Table 3 provides the results of the ten ANN models created for the purpose of cross-validation. The average Root Mean Square Error (RMSE) values for the training and testing phases are 0.2494 and 0.2972, respectively. With these values falling under 0.5, it suggests a strong fit for the model. The correlation between the predicted and observed values for each model, as included in Table 3, returns an average R square value of 0.84. This indicates the model's ability to predict TDS with an accuracy of 84%. Figure 2 shows the plotted RMSE values for the ten generated Multilayer Perceptron-ANN (MLP-ANN) models, both for training and testing, demonstrating promising results.

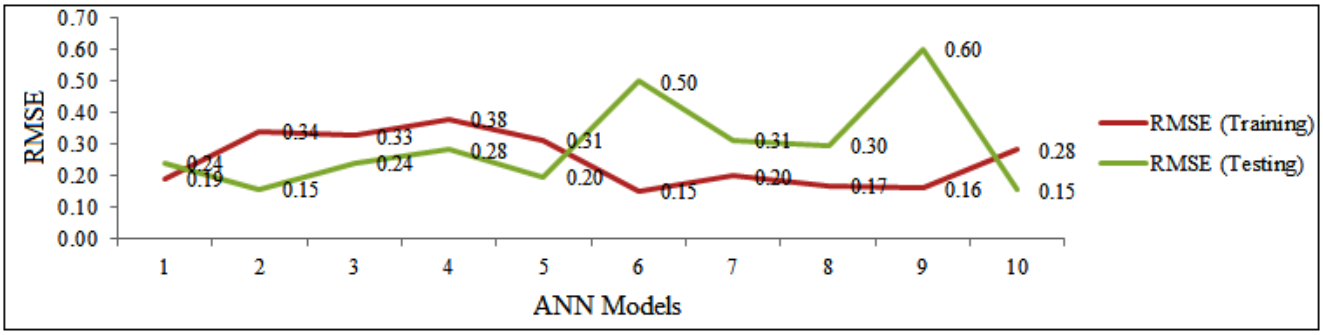

Fig 2 RMSE of Training and Testing Models for NAS

Table 3 Result Summary of ANN Model for NAS

Training				Testing				
N	Network	Sum of square error (Training)	RMSE (Training)	N	Sum of square error	Root mean square of errors	Total samples	R square of Predicted Vs Observed TDS
36	1	1.272	0.1879	14	0.809	0.2403	50	0.90
38	2	4.385	0.3396	12	0.286	0.1543	50	0.80
34	3	3.605	0.3256	16	0.923	0.2401	50	0.79
32	4	4.588	0.3786	18	1.421	0.2809	50	0.76
38	5	3.688	0.3115	12	0.461	0.1960	50	0.83
35	6	0.766	0.1479	15	3.722	0.4981	50	0.88
34	7	1.324	0.1973	16	1.551	0.3113	50	0.89
32	8	0.902	0.1678	18	1.577	0.2959	50	0.88
37	9	0.918	0.1575	13	4.718	0.6024	50	0.83
35	10	2.751	0.2803	15	0.35	0.1527	50	0.87
	Mean	2.420	0.2494	Mean	1.582	0.2972		0.84
	Std Dev	1.546	0.0865	Std Dev	1.4879	0.1460		

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Sensitivity analysis allows us to determine the predictive strength and importance of each input neuron in the ANN model. The normalised importance of input neurons is calculated by dividing the relative importance of each neuron by the maximum neuron [19]. Table 4 reveals that in predicting TDS, the order of importance is as follows: sulphate (100%), bicarbonate (89.39%), sodium (79.48%), chloride (66.85%), magnesium (49.96%), location (40.89%), months (37.53%), potassium (31.56%), calcium (18.53%), and carbonate (15.31%). It can be concluded that sulphate, originating from anthropogenic activities, is the strongest predictor for TDS in the NAS. The dominance of sulphate also indicates the source of groundwater as an intermediate recharge zone. Sampling locations and months have a negligible impact on TDS prediction in this context.

Table 4 Results of Sensitivity Analysis for NAS

Neural networks	Locations	Months	Calcium	Magnesium	Sodium	Potassium	Carbonate	Bicarbonate	Chloride	Sulphate
NN 1	0.342	0.41	0.24	0.35	0.84	0.35	0.29	0.99	0.52	1.00
NN 2	0.337	0.18	0.03	0.39	0.49	0.12	0.11	0.74	0.72	1.00
NN 3	0.285	0.29	0.34	0.56	0.40	0.31	0.12	1.00	0.63	0.29
NN 4	0.248	0.30	0.07	1.00	0.94	0.62	0.10	0.62	0.68	0.65
NN 5	0.219	0.36	0.03	0.42	0.72	0.15	0.08	0.33	0.37	1.00
NN 6	0.37	0.31	0.14	0.12	0.56	0.14	0.25	0.79	0.50	1.00
NN 7	0.391	0.37	0.27	0.47	0.81	0.14	0.07	0.71	0.78	1.00
NN 8	0.306	0.23	0.14	0.10	0.46	0.32	0.10	0.68	0.31	1.00
NN 9	0.659	0.35	0.25	0.56	0.95	0.39	0.12	1.00	0.63	0.44
NN 10	0.27	0.34	0.04	0.22	0.49	0.09	0.05	0.62	0.46	1.00
Average Importance	0.34	0.31	0.16	0.42	0.67	0.26	0.13	0.75	0.56	0.84
Normalised importance	40.89%	37.53%	18.53%	49.96%	79.48%	31.56%	15.31%	89.39%	66.85%	100.00%
Ranking	6	7	9	5	3	8	10	2	4	1

For SAS, applying the same ten-fold cross-validation process of MLP, we observe an average RMSE of 0.2 and 0.363 for training and testing, respectively (Table 5). The standard deviation of RMSE is 1.546 and 0.1469 for training and testing. The mean R square value for observed versus predicted is 0.853. Figure 3 shows the plot of the RMSE training and testing values against the models, visually indicating the validity of the ten models used in the ANN cross-validation.

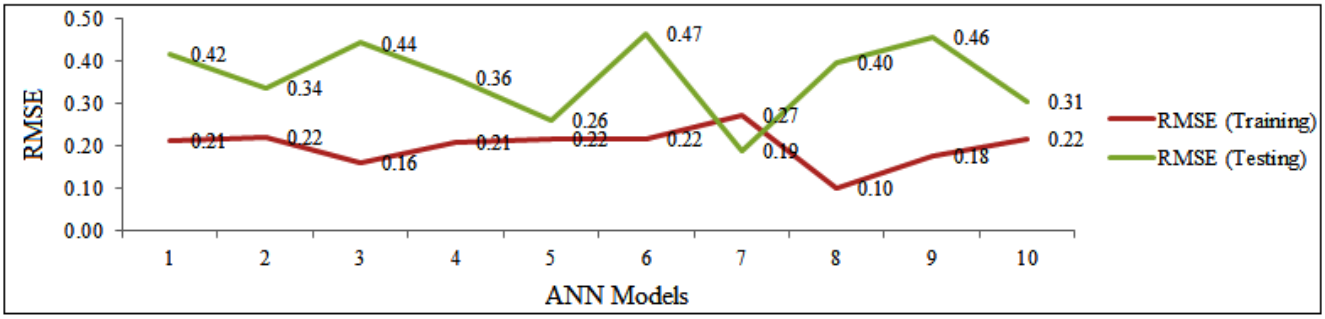

Fig 3 RMSE of Training and Testing Models for SAS.

Table 5 Result Summary of ANN Model for SAS

Training(				Testing				
N	Network	Sum of square error (Training)	RMSE (Training)	N	Sum of square error	Root mean square of errors	Total samples	R square of Predicted Vs Observed TDS
36	1	1.634	0.2130	14	2.438	0.4173	50	0.841
38	2	1.835	0.2197	12	1.355	0.3360	50	0.864
34	3	0.878	0.1606	16	3.134	0.4425	50	0.831
32	4	1.369	0.2068	18	2.352	0.3614	50	0.823
38	5	1.766	0.2155	12	0.814	0.2604	50	0.892
35	6	1.632	0.2159	15	3.238	0.4646	50	0.824
34	7	2.539	0.2732	16	0.569	0.1885	50	0.871
32	8	0.323	0.1004	18	2.848	0.3977	50	0.863
37	9	1.137	0.1752	13	2.707	0.4563	50	0.858
35	10	1.616	0.2148	15	1.397	0.3051	50	0.87
	Mean	1.4729	0.20		2.0852	0.363		0.853
	Std Dev	0.5986	0.046		0.9726	0.091		0.023

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The sensitivity analysis helps to assess the predictive strength of input neurons. As outlined in Table 6, the sensitivity analysis results for the ten-fold cross-validation ANN for SAS show that the normalised importance percentages suggest that TDS predictability is primarily controlled by sodium (100%), magnesium (87.74%), potassium (66.69%), Chloride (51.23%), Sulphate (47.11%), location (41.90%), bicarbonate (33.81%), calcium (29.17%), month (24.71%), and carbonate (15.32%).

Table 6 Result Summary of Sensitivity Analysis for SAS

Neural networks	Locations	Months	Calcium	Magnesium	Sodium	Potassium	Carbonate	Bicarbonate	Chloride	Sulphate
NN 1	0.30	0.07	0.018	0.54	1	0.51	0.25	0.21	0.2	0.13
NN 2	0.44	0.4	0.47	0.5	0.66	1	0.08	0.57	0.9	0.77
NN 3	0.348	0.264	0.075	0.782	1	0.501	0.084	0.162	0.43	0.472
NN 4	0.444	0.274	0.317	0.701	0.707	1	0.261	0.289	0.489	0.147
NN 5	0.788	0.334	0.358	0.626	1	0.479	0.095	0.878	0.604	0.643
NN 6	0.283	0.152	0.445	1	0.761	0.183	0.096	0.163	0.137	0.844
NN 7	0.198	0.109	0.157	0.621	1	0.329	0.169	0.094	0.164	0.458
NN 8	0.294	0.181	0.278	0.725	1	0.509	0.122	0.262	0.041	0.24
NN 9	0.235	0.113	0.102	1	0.648	0.325	0.133	0.115	0.833	0.085
NN 10	0.252	0.21	0.272	1	0.766	0.861	0.019	0.145	0.578	0.235
Average Importance	0.36	0.21	0.2492	0.7495	0.8542	0.5697	0.1309	0.2888	0.4376	0.4024
Normalised importance	41.90%	24.71%	29.17%	87.74%	100.00%	66.69%	15.32%	33.81%	51.23%	47.11%
Ranking	6	9	8	2	1	3	10	7	4	5

IV. CONCLUSION

Comparing the regression models for the Northern Area Samples (NAS) and Southern Area Samples (SAS) reveals distinctive controlling variables within these two geographically separate locations over the same periods. The primary differentiating factor between these two sets of sampling locations is the presence of a township. In the NAS, sodium, bicarbonate, and chloride serve as major predictors, while in the SAS, magnesium and sodium are more influential.

The presence of bicarbonate in NAS is indicative of groundwater that has travelled a short distance after recharge. Sodium enters the system and displaces calcium and magnesium from the subsoil, thus releasing them into the groundwater, suggesting an ion-exchange reaction. The heightened sodium levels can escalate soil salinity, potentially undermining crop yields. This phenomenon aligns with field observations noting soil salinity issues in patches southeast of the town.

The Artificial Neural Network (ANN) models for both the NAS and SAS datasets demonstrate robustness and strong validity, boasting high R square values between observed and predicted neurons. The calculated Root Mean Square Error (RMSE) for both NAS and SAS models is less than 0.5 for both the training and testing validation phases, underlining the reliability of the models.

The Multilayer Perceptron (MLP) models highlight the strong predictive strength of input neurons for both the NAS and SAS. Sensitivity analysis and subsequent ranking transformation of variables for NAS indicate that sulphate, bicarbonate, sodium, and chloride are dominant TDS predictors in the model. For SAS, the key TDS predictors are sodium, magnesium, potassium, and chloride. The prevalence of chloride in the SAS signals anthropogenic influence and the existence of a regional discharge zone.

Interestingly, MLP models yield better predictive results for TDS than the regression models, demonstrating their broader utility for predictive modelling and groundwater quality characterisation. In conclusion, ANN predictive models for TDS provide more accurate results than multilayer regression models. Thus, ANNs can serve as not only a tool for predictive modelling but also a superior approach for hydrochemical characterisation.

It is interesting to note that for both NAS and SAS, location and month showed a lesser degree of influence on the TDS prediction. These findings provide a valuable understanding of groundwater quality and can guide effective management strategies to maintain the sustainability of this vital resource in areas that rely heavily on groundwater. Further studies could extend these models to predict other groundwater quality parameters or apply them to different regions or environmental contexts. Additionally, it could be beneficial to explore the effects of different anthropogenic activities on groundwater quality more explicitly. Lastly, incorporating temporal changes in these models could yield insightful results, capturing seasonal variations in groundwater quality.

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